

1,1-dimethoxyhexan-2-one
6344-10-1 | DTXSID70287285

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 8.69e-01

Global applicability domain: Inside

Local applicability domain index: 5.45e-01

Confidence level: 7.48e-01

Nearest Neighbors from the Training Set

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2-(2-Butoxyethoxy)ethanol

Measured: 0.56

Predicted: 5.85e-01

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Butyl glycidyl ether

Measured: 0.63

Predicted: 7.76e-01

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Acetal

Measured: 0.84

Predicted: 8.05e-01

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2-[2-(Hexyloxy)ethoxy]ethanol

Measured: 1.70

Predicted: 1.54

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Diethoxymethane

Measured: 0.84

Predicted: 6.96e-01